Overview of NASA QuAIL team research and Introduction to Quantum Computing

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IARPA
BE THE FUTURE

QUANTUM ENHANCED OPTIMIZATION

23 January 2020 **NASA Ames Research Center**

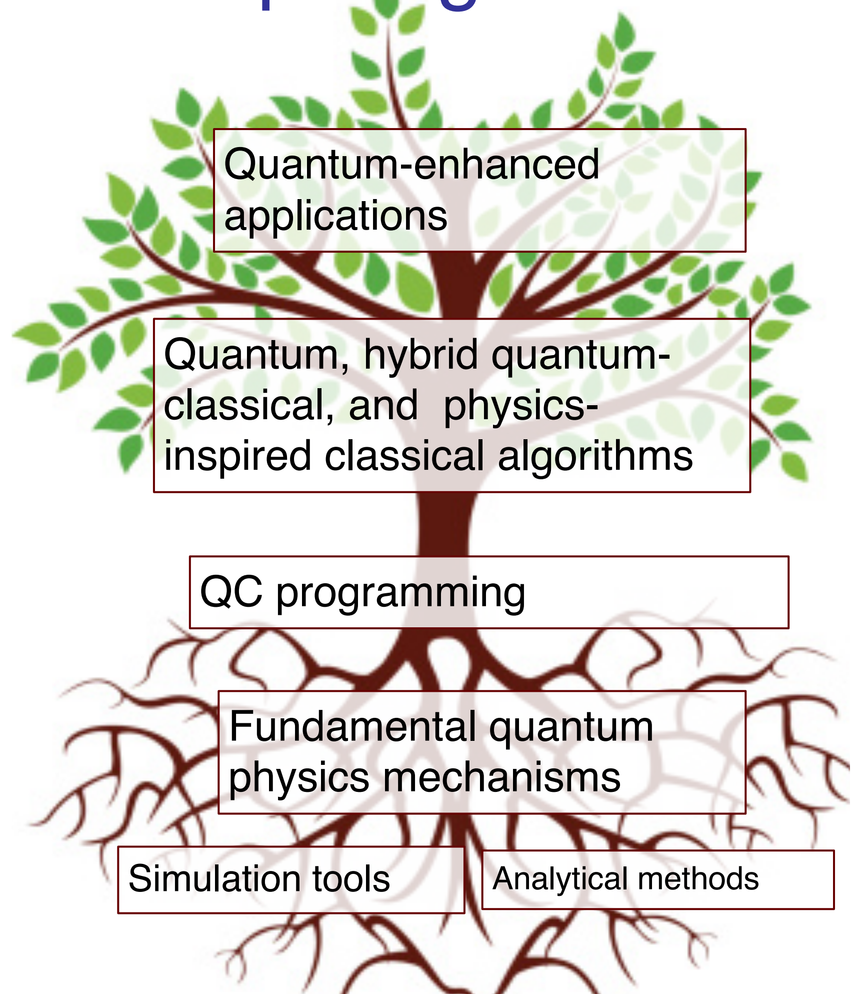
NASA's Stake in Quantum Computing

NASA constantly confronting massively challenging computational problems

- Computational capacity limits mission scope and aims

NASA's Pleiades
One of the top 25 fastest supercomputers in the world

NASA QuAIL mandate:
Determine the potential for quantum computation to enable more ambitious and safer NASA missions in the future



NASA Ames QuAIL team

Quantum Computing in one slide

Pool of quantum properties

- Quantum interference
- Quantum entanglement
- Quantum tunneling
- Quantum sampling
- Quantum measurement
- Non-commutative quantum operators
- Quantum population transfer
- Quantum many-body delocalization
- Quantum no cloning theorem
- Quantum adiabatic theorem
- Quantum discord

The power of quantum computation comes from encoding information in a non-classical way

Quantum computers take advantage of quantum effects not available classically

These effects can provide more efficient computation and higher levels of security than is available classically

What Shor's factoring algorithm can compute in days, would take a supercomputer longer than the age of the universe

Breaks all public key encryption in standard use

The art of quantum algorithm design is figuring out how to harness peculiarly quantum properties for computational purposes

Outline of talk

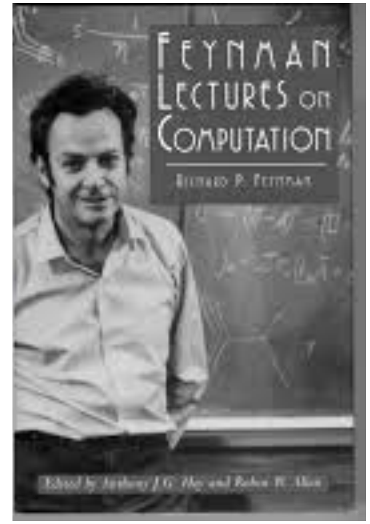
Part I: High-level discussion of quantum computing

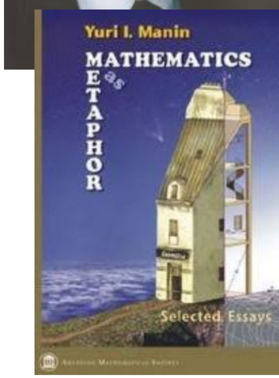
Part II: Basic concepts in quantum computing

Part III: NASA QuAIL Research Overview

Birth of quantum computing

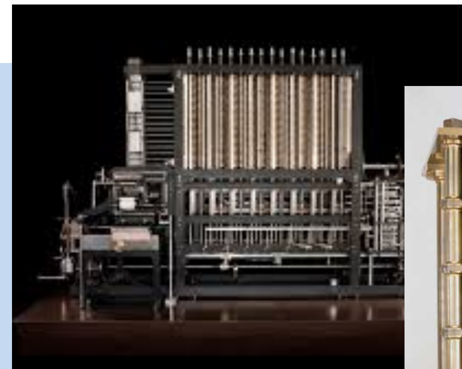
- Feynman and Manin recognized in the early 1980s that certain quantum phenomena could not be simulated efficiently by a computer
  - Phenomena related to quantum entanglement; Bell’s inequality
  - Reason materials are hard to simulate at the quantum level
- Perhaps these quantum phenomena could be used to speed up more general computation?



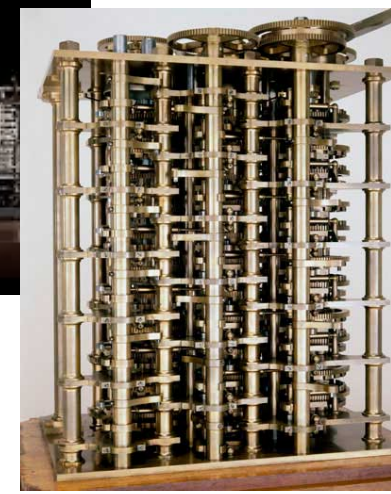


Computers as classical mechanical machines

- Babbage's analytical engine was a classical mechanical machine
- Turing machines
  - The abstraction that underlies complexity theory and universal computing machines
  - Firmly rooted in classical mechanics
  - Described in classical mechanical terms



Babbage engine (Computer History Museum)



- Abstraction allowed us ignore how classical computers are implemented physically
  - When we program we don't think about the fundamental physics
- ***How do different models of physics affect how quickly we can compute***

What a quantum computer is not

- **Just because a computer uses quantum effects, does not mean it is a quantum computer**
  - All the computers in this building make use of quantum effects
  - The fundamental unit of computation, the bit, and the algorithms we design for computers did not change when quantum effects were used
- **A quantum computer has a fundamentally different way of encoding and processing information**
  - Quantum computers are quantum information processing devices
  - They process qubits instead of bits
  - They use quantum operations instead of logic gates
- **Also, just because a piece of hardware has a certain number of qubits, it isn't necessarily a quantum computer**
  - A set of light switches, even a very large set, is not a classical computer

Certainty and randomness in quantum computation

- Any computation a classical computer can do, and quantum computer can do with roughly the same efficiency
  - With the same probability of the outcome
  - if the classical computation is non-probabilistic, so is the quantum one
- Like classical algorithms, some quantum algorithms are inherently probabilistic and others are not
  - First quantum algorithms were not probabilistic
    - E.g. Deutsch-Jozsa algorithm solves problem with certainty that classical algorithms, of equivalent efficiency, could solve only with high probability
  - Shor's algorithms are probabilistic
  - Grover's is not intrinsically probabilistic
    - initial search algorithm was probabilistic, but
    - slight variants, which preserve the speed up, are non-probabilistic

Current status of quantum algorithms

Quantum computing can do everything a classical computer can do

and

Provable quantum advantage known for a few dozen quantum algorithms

Unknown quantum advantage for everything else

Status of classical algorithms

- Provable bounds hard to obtain
  - Analysis is just too difficult
- Best classical algorithm not known for most problems
- Empirical evaluation required
- Ongoing development of classical heuristic approaches
  - Analyzed empirically: ran and see what happens
  - E.g. SAT, planning, machine learning, etc. competitions

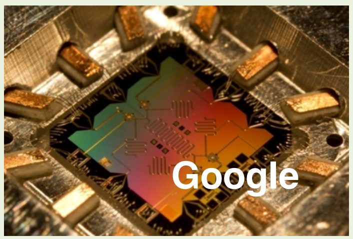
- **NISQ era supports unprecedented means for empirical analysis of quantum algorithms**
  - **Quantum heuristics come into their own**

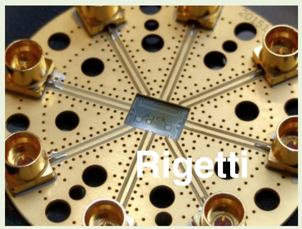
A handful of proven limitations on quantum computing

Conjecture: Quantum Heuristics will significantly broaden applications of quantum computing

Quantum hardware

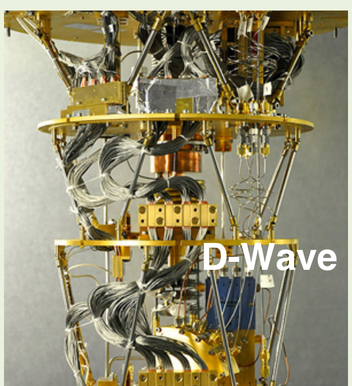
General Purpose:
Universal quantum processors





Special Purpose:
E.g. Quantum annealers

Noisy Intermediate-Scale Quantum (NISQ) devices



Superconducting processors
- ***Google, IBM, Rigetti, Intel, …***

Trapped ion processors
- ***IonQ, Honeywell, …***

Other approaches
- **Optical**
- **Electron spins in silicon**
- **Topological, anyon based quantum computing**

Number of qubits alone is not a good measure
- **Analogy: billions of switches do not a classical computer make**

Other key factors
- **precision, speed, and generality of the control**
  - **particularly operations involving multiple qubits**
- **how long quantum coherence can be maintained**
- **stability over time**
- **speed with which processors can be calibrated**

National Aeronautics and Space Administration

Ames

Discovery · Innovations · Solutions

Quantum computing has entered the NISQ Era

Quantum supremacy has been achieved!

- Perform computations not possible on even the largest supercomputers


Article

Quantum supremacy using a programmable superconducting processor

Cover article, Nature, 24 Oct 2019

Google, NASA, ORNL collaboration

https://www.nature.com/articles/s41586-019-1666-5

https://www.nasa.gov/feature/ames/quantum-supremacy

… but not <u>useful</u> quantum supremacy.

- Currently too small to be useful for solving practical problems
- Early application to certified random number generation, but other applications require larger, more capable devices

Uses of these still limited, quantum devices?

(1) Unprecedented opportunity to explore and **evaluate algorithms**, both quantum and hybrid quantum-classical heuristic algorithms

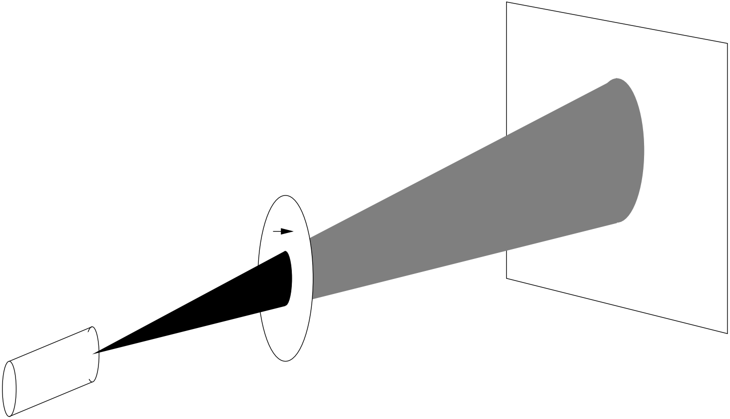
(2) Investigate quantum mechanisms that may be harnessed for computational purposes

Insights gained feed into next generation

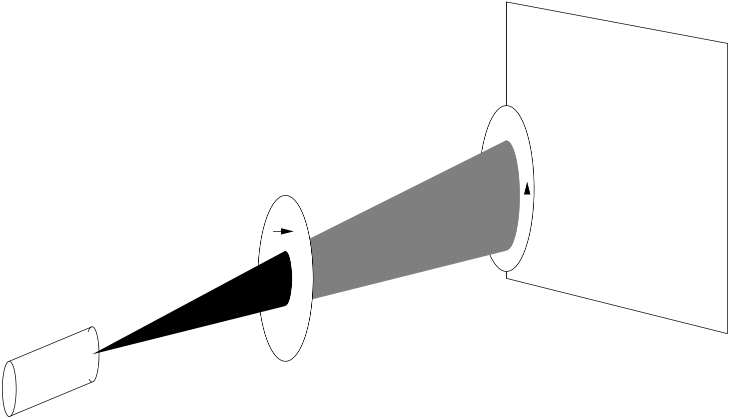
- **quantum algorithms**
- **quantum hardware**

Early target: Optimization; Sampling & Machine Learning; simulation of quantum systems

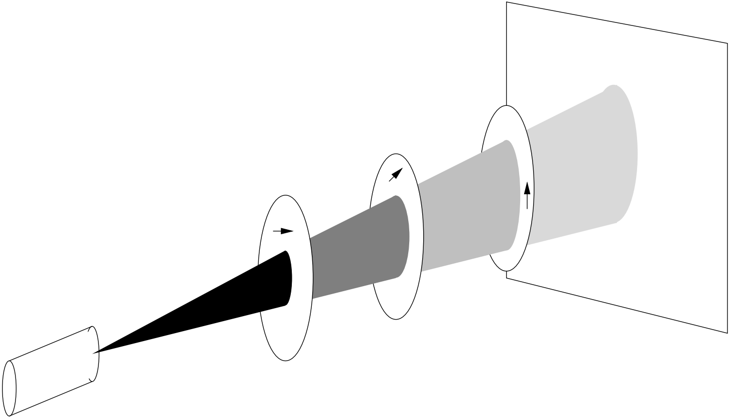
A simple experiment: photon polarization



A simple experiment: photon polarization



A simple experiment: photon polarization



Photon Polarization

Polarization state of a photon

- can be represented as a 2-dimensional vector of unit length

Taking horizontal $|\rightarrow\rangle$ and vertical $|\uparrow\rangle$ polarizations as a basis, an arbitrary polarization can be expressed as a superposition

$$|\psi\rangle = a|\uparrow\rangle + b|\rightarrow\rangle$$

with $|a|^2 + |b|^2 = 1$

(Allowing a and b to be complex numbers enables this formalism to describe circular polarization as well)

$|v\rangle$ is Dirac's notation for vectors. Means the same thing as $\vec{v}$ or $\mathbf{v}$, with v being the label for the vector

Measurement of polarization

Polarization filters are quantum measuring devices

Quantum measurements always occur w.r.t. an orthogonal subspace decomposition associated with the measuring device

For a horizontal polarization filter, the basis in which it measures is $|\rightarrow\rangle$, together with its perpendicular $|\uparrow\rangle$

A photon with polarization $a|\uparrow\rangle + b|\rightarrow\rangle$ is measured by a horizontal filter as $|\uparrow\rangle$ (absorbed) with probability $|a|^2$, and
$|\rightarrow\rangle$ (passed) with probability $|b|^2$

Any photon that has passed through the filter now has polarization $|\rightarrow\rangle$.

Polarization filters at other angles work in a similar way

Quantum bits, or qubits

Think polarization states of a photon!

Any 2-dimensional quantum system can be viewed as the fundamental unit of quantum computation, a *quantum bit* or *qubit*.
Qubit state space is a 2-dimensional complex vector space

A computational basis is chosen, denoted $|0\rangle$ and $|1\rangle$, and used to encode classical bit values 0 and 1

Possible qubit values $a|0\rangle + b|1\rangle$, for complex a, b with $|a|^2 + |b|^2 = 1$.

Unlike classical bits, qubits can be in superposition states such as $\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ or $\frac{1}{\sqrt{2}}(|0\rangle - i|1\rangle)$

How State Spaces Combine

Let X be a vector space with basis $\{|\alpha_1\rangle, \ldots, |\alpha_n\rangle\}$ and Y be a vector space with basis $\{|\beta_1\rangle, \ldots, |\beta_m\rangle\}$

Classical state spaces combine via the **Cartesian product**

$X \times Y$ has basis $\{|\alpha_1\rangle, \ldots, |\alpha_n\rangle, |\beta_1\rangle, \ldots, |\beta_m\rangle\}$

$$\begin{aligned} \dim(X \times Y) &= \dim(X) + \dim(Y) \\ &= n + m \end{aligned}$$

Quantum state spaces combine via the **tensor product**

$X \otimes Y$ has basis $\{|\alpha_1\rangle \otimes |\beta_1\rangle, |\alpha_1\rangle \otimes |\beta_2\rangle, \ldots, |\alpha_n\rangle \otimes |\beta_m\rangle\}$

$$\begin{aligned} \dim(X \otimes Y) &= \dim(X) * \dim(Y) \\ &= n * m \end{aligned}$$

Entangled states

Entangled states cannot be written as tensor product of independent qubits

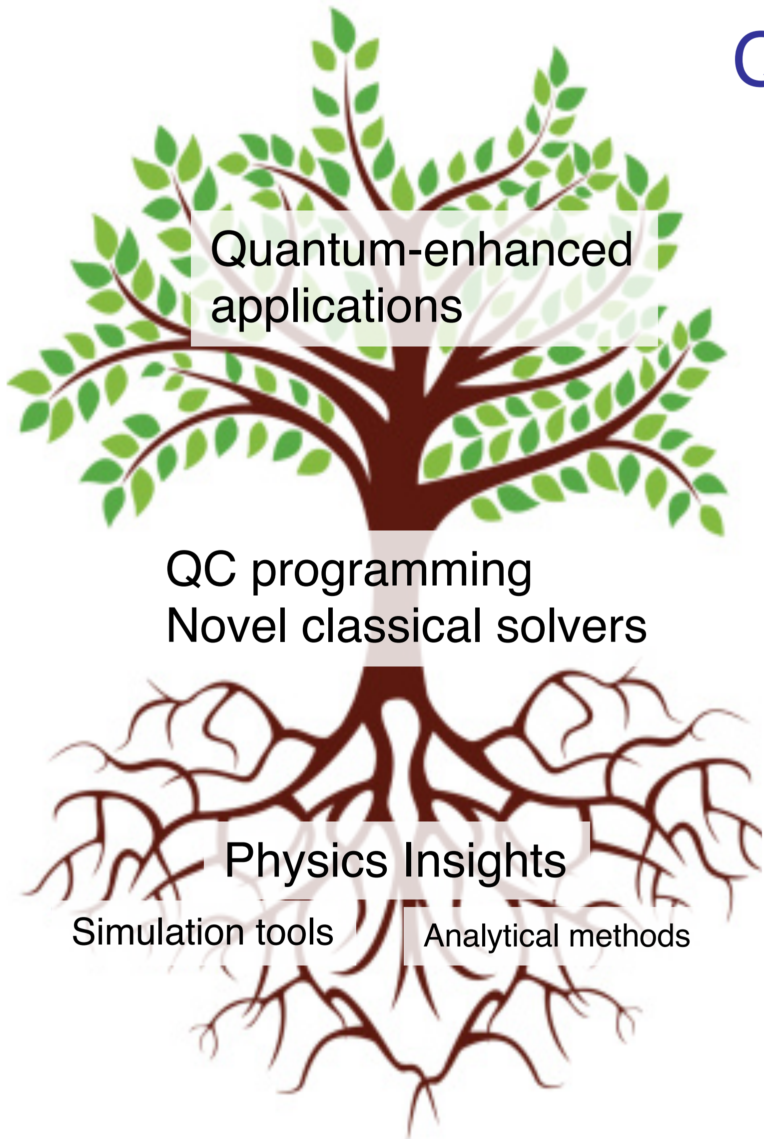
Example: An EPR pair $\frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$

$$\begin{aligned}
& (a_0|0\rangle + b_0|1\rangle) \otimes (a_1|0\rangle + b_1|1\rangle) \\
= \quad & a_0 a_1|00\rangle + a_0 b_1|01\rangle + b_0 a_1|10\rangle + b_0 b_1|11\rangle \\
\neq \quad & a_0 a_1|00\rangle + 0|01\rangle + 0|10\rangle + b_0 b_1|11\rangle \\
= \quad & \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)
\end{aligned}$$

- Measurement of the first qubit yields either $|0\rangle$ or $|1\rangle$
- Measurement changes state to either $|00\rangle$ or $|11\rangle$
- Measurement of second qubit gives same result as first

Similar results when measuring in other bases

Quantum Computing at NASA



Application focus areas

- **Planning and scheduling**
- **Robust networks**
- **Fault Diagnosis**
- **Machine Learning**
- **Material science simulations**

Programming quantum computers

- **Quantum algorithm design**
- **Mapping, parameter setting, error mitigation**
- **Hybrid quantum-classical approaches**
- **Compiling quantum algorithms to hardware**

QC → state-of-the-art classical solvers

Physics insights into quantum algorithm and quantum hardware design

Quantum Optimization Algorithms: AQO, QA, QAOA

Common elements: Given cost function C(z),

- **Phase separation operator based on the cost function,**

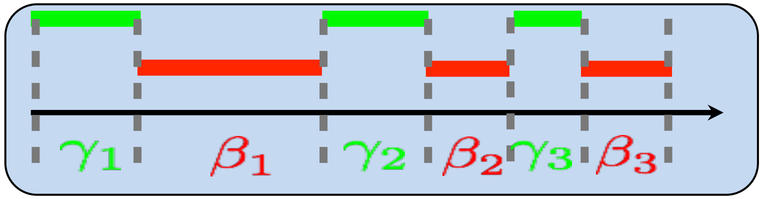
  Usually based on $H_P = -C(z)|z\rangle\langle z|$, often including additional "penalty terms" to enforce constraints

- **Driver/Mixing operator**

  Most frequently $H_M = \sum_j X_j$, though we will shortly see other mixers

AQO	**QA**	**QAOA**
• Evolution under $\boldsymbol{H(t) = a(t)}H_P + \boldsymbol{b(t)}H_M$ • Slowly enough to stay in the ground subspace	• Evolution under $\boldsymbol{H(t) = a(t)}H_P + \boldsymbol{b(t)}H_M$ • Many quick runs, thermal effect contribute	• Alternate application of H_P and H_M • For $\boldsymbol{p}$ alterations, the parameters are $\boldsymbol{2p}$ times/angles $\boldsymbol{\gamma_1, \beta_1, \ldots \gamma_P, \beta_p}$

QAOA



Based on the Quantum Approximate Optimization Algorithm

- A gate model heuristic due to Farhi et al.
- Iterates between two Hamiltonians, p times, applied for times β_i and γ_i
  - Phase separation (encodes cost function)
  - Mixing

Early results by Farhi and co-authors

- p → ∞: from AQO
  - Converges to optimum for p → ∞
- p = 1: from IQP circuits
  - Provably hard to sample output efficiently classically (up to standard complexity theory conjectures)
  - Beat existing classical approximation ratio on MaxE3Lin2 only to inspire a better classical algorithm

Quantum Alternating Operator Ansatz, generalizing Farhi et al., QAOA

- More general mixing operators

- Inspired by compilation concerns, thus enabling earlier evaluation on nearer-term hardware

- Incorporates hard constraints into mixer instead of as a penalty term

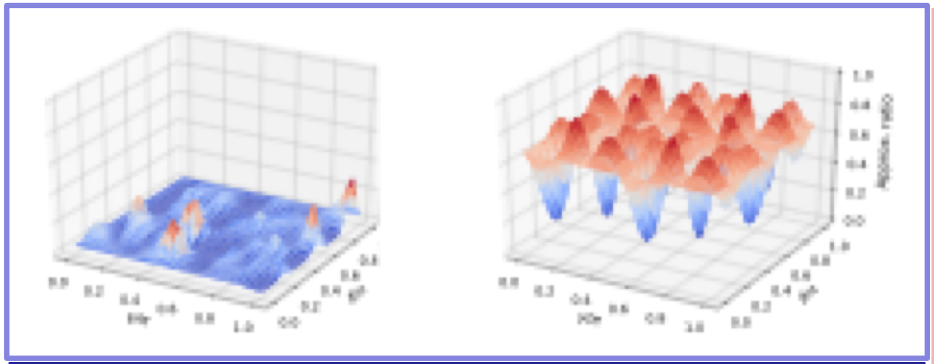
Algorithm explores only feasible subspace, often exponentially smaller, so more efficient search

Wang, Rubin, Dominy, Rieffel. **XY mixer for QAOA on graph coloring problems**. *(To appear)*

We have mapped many optimization problems to the QAOA formalism

S. Hadfield et al., **From the Quantum Approximate Optimization Algorithm to a Quantum Alternating Operator Ansatz,** *Algorithms 12 (2), 34 2019*

Advantage of XY-mixer



Numerical results: approximation ratio for 3-coloring a triangle (Left) QAOA with std X-mixer. (Right) QAOA with XY-mixer

Confirmed advantage of mixers that maintain evolution within feasible subspace

- Exponentially smaller subspace, but still exponentially large
- Ratio shrinks exponentially with n:
- - $$\frac{\dim(\mathcal{H}_{\mathrm{fea}})}{\dim(\mathcal{H})} = \frac{\kappa^n}{2^{n\kappa}} = \left(\frac{\kappa}{2^\kappa}\right)^n$$

Zhihui Wang, Nicholas C. Rubin, Jason M. Dominy, Eleanor G. Rieffel, **XY-mixers: analytical and numerical results for QAOA,** *arXiv:1904.09314*

Parameter setting

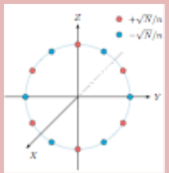
New algorithm for Grover's problem

- QAOA circuit O(√N) query complexity

- Trotterizing Roland-Cerf loses O(√N) q.c.

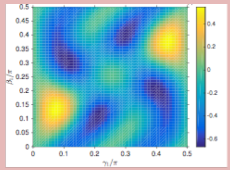
- Demonstrates utility of periodic parameters

- Coherent state analysis



Jiang, Rieffel, Wang, **Near-optimal quantum circuit for Grover's unstructured search using a transverse field**. *PRA* (2017)

Analysis of QAOA on ring



- Mapping to Jordan-Wigner

- Explains parameter symmetries

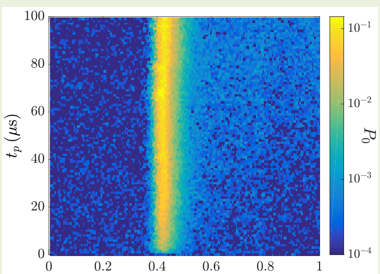
- Provides orders of magnitude more efficient numerical investigation

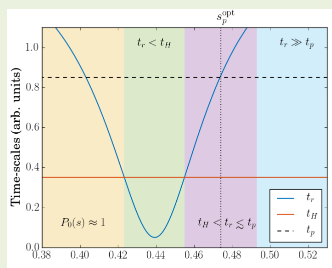
Wang, Hadfield, Jiang, Rieffel. **QAOA for MaxCut: A Fermionic View**. *PRA* (2018)

Example investigations of quantum mechanisms

The Power of Pausing

Pausing at good time in anneal increases performance by orders of magnitude





Correct model of annealing required.

Pause effective where thermalization slows (rather than at minimum gap)

Collaboration: Illustrates effective feeding of information into quantum hardware design from users and theorists

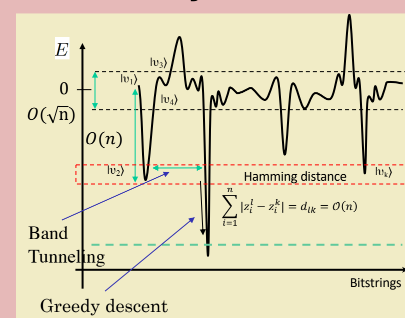
J. Marshall, D. Venturelli, I. Hen, E. Rieffel, **The power of pausing: advancing understanding of thermalization in experimental quantum annealers**, accepted *Phys Rev Applied*, 2019

Harnessing quantum MBDL for quantum computation

Hybrid opt. alg.: Quantum band tunneling combined with greedy descent

- Obtain square-root speed up in random energy model

- Totally different mechanism than Grover



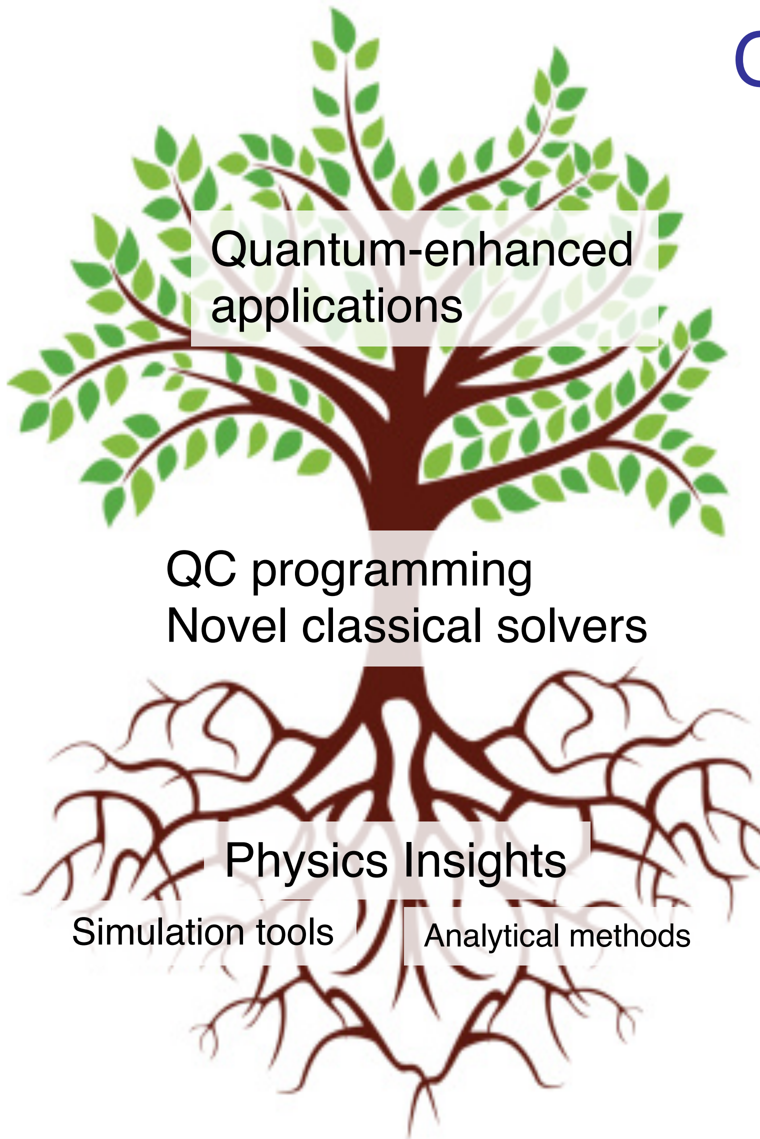
*Key concept: **Band Tunneling** induced by quantum many-body delocalization (MBDL). Population transfer occurs within a network of resonances*

Collaboration with Google

K. Kechedzhi et al., **Efficient population transfer via non-ergodic extended states in quantum spin glass**, arXiv:1807.04792

V. Smelyanskiy et al., **Non-ergodic delocalized states for efficient population transfer within a narrow band of the energy landscape**, arXiv:1802.09542

Quantum Computing at NASA



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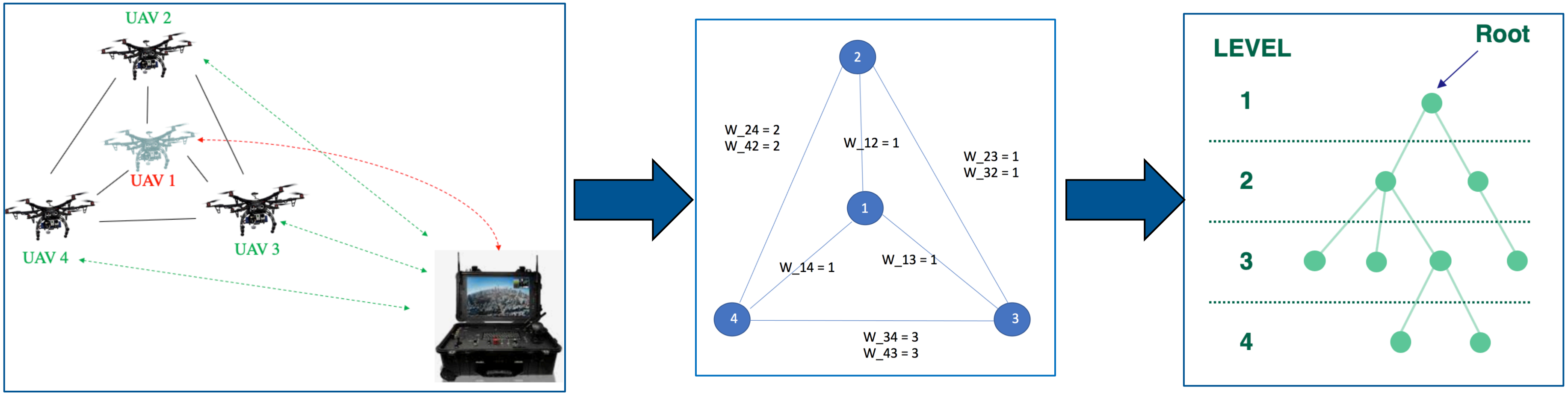
Robust Communication Network Design

Future of air traffic

- Higher vehicle density
- Heterogeneous vehicles
- Mixed equipage
- Greater autonomy

Challenge: assure communication availability



Surrogate problem: minimum weighted spanning tree with degree constraints

Pause shift for degree bounded spanning trees

Robust communications networks

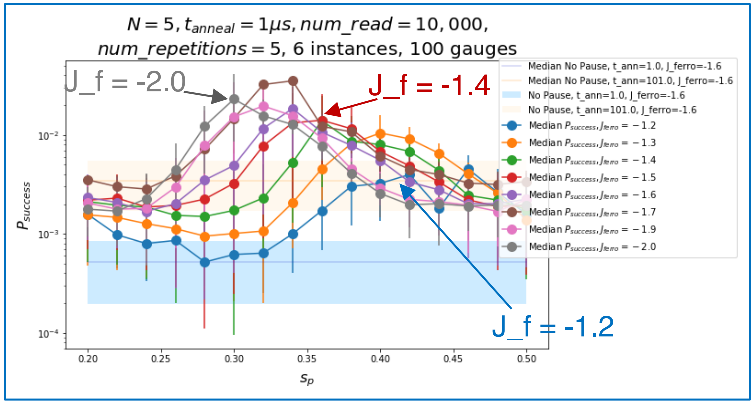
- **assuring communication availability**
- **essential for airspace with increasing vehicle density and diversity including small Unmanned Aerial Systems (sUAS)**

surrogate problem: minimum degree-bounded spanning tree within a communications graph

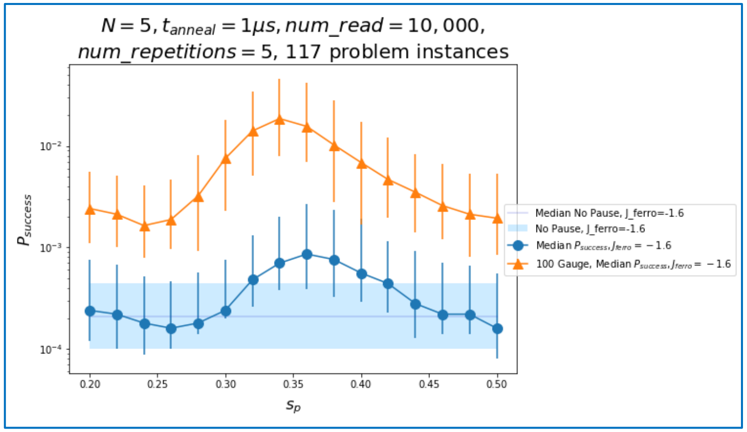
Demonstrated effectiveness of an annealing pause on these instances

- **confirmed pause on embedded instances demonstrated,**
- **confirmed theory that pause location shift earlier in anneal with increasing ferromagnetic coupling**

Effectiveness of partial gauge transformation for hardware with asymmetric parameter ranges



Shift in the best pause location with increasing J_f
Probability of success (y-axis) pause location (x-axis)



Effect of 100 partial gauges on $P_{success}$ with J_f = -1.6

Simulating quantum systems

Quantum Simulation is one of the important applications we expect to run on quantum computers.

Elucidating Reaction Mechanisms on Quantum Computers

Markus Reiher,[1] Nathan Wiebe,[2] Krysta M. Svore,[2] Dave Wecker,[2] and Matthias Troyer[3,2,4]

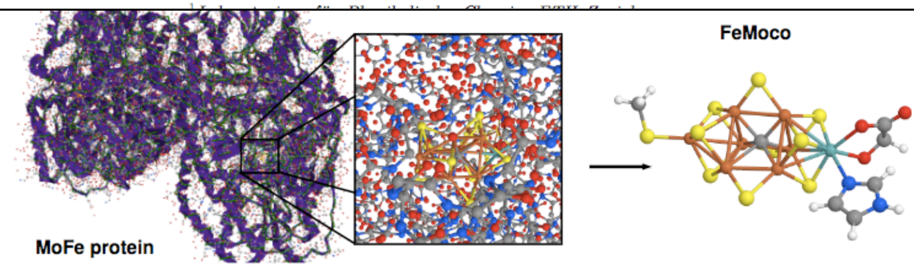


FIG. 1. X-ray crystal structure 4WES [21] of the nitrogenase MoFe protein from *Clostridium pasteurianum* taken from the protein data base (left; the backbone is colored in green and hydrogen atoms are not shown), the close protein environment of the FeMoco (center), and the structural model of FeMoco considered in this work (right; C in gray, O in red, H in white, S in yellow, N in blue, Fe in brown, and Mo in cyan).

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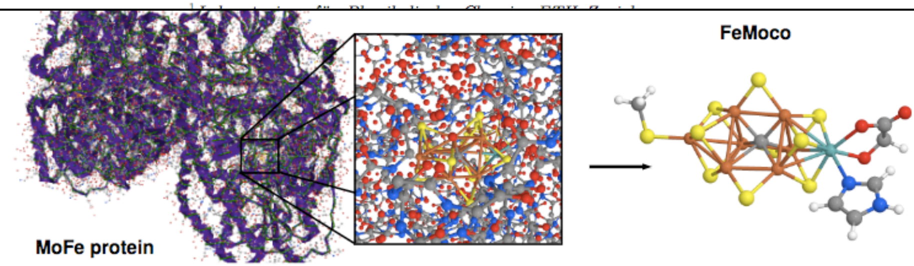

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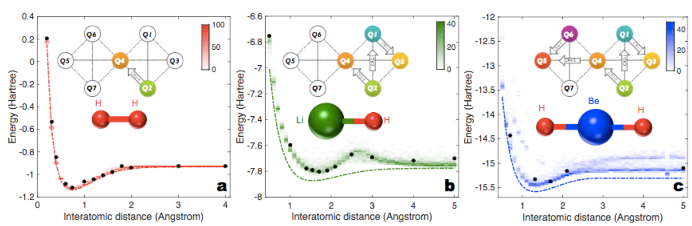
There are two popular algorithms that have been suggested for quantum simulation:

1) Variational Quantum Eigensolver (similar to variational Monte Carlo)
2) Phase Estimation (An algorithm based on time evolution)



Hardware-efficient Variational Quantum Eigensolver for Small Molecules and Quantum Magnets

Abhinav Kandala,* Antonio Mezzacapo,* Kristan Temme, Maika Takita, Markus Brink, Jerry M. Chow, and Jay M. Gambetta
IBM T.J. Watson Research Center, Yorktown Heights, NY 10598, USA
(Dated: October 16, 2017)

The need for high fidelity wave functions

Good wave functions are needed for virtually all quantum algorithms. High overlap with ground states needed for **phase estimation**. Even higher needed for **VQE,** although optimization is possible with a quantum computer.

$$|\psi_{\text{in}}\rangle = \sum_{\ell=1}^{L} \alpha_\ell \,|D_\ell\rangle$$

The full wavefunction has exponential number of degrees of freedom.

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Good wave functions are needed for virtually all quantum algorithms. High overlap with ground states needed for **phase estimation**. Even higher needed for **VQE**.

$$|\psi_{\rm in}\rangle = \sum_{\ell=1}^{L} \alpha_\ell \, |D_\ell\rangle$$

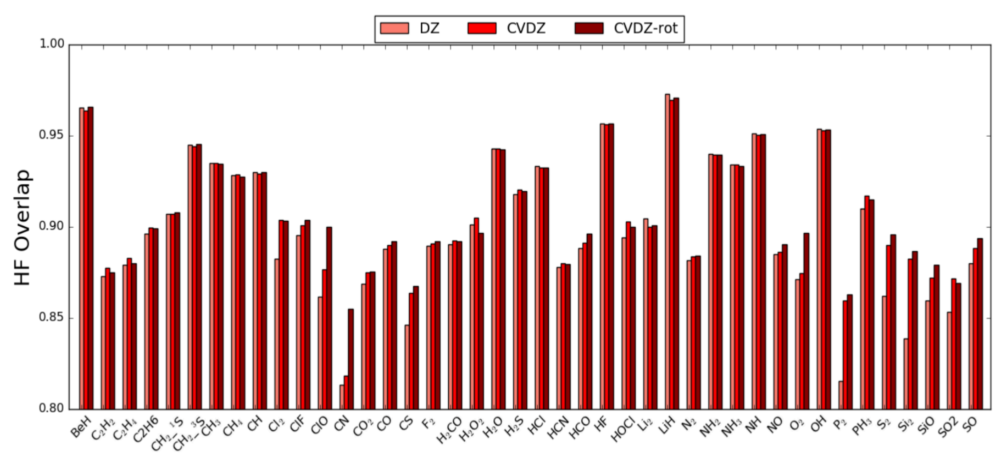
The full wavefunction has exponential number of degrees of freedom.

Overlap/Fidelities for 55 molecules

What are good algorithms for generating wave functions (created classically) on quantum computers?

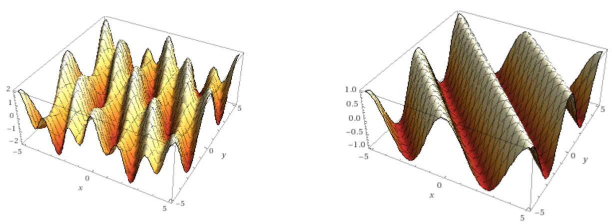
G2 Set of 55 molecules. Includes (molecules consisting of C,N,H,SI,O).

Hartree-Fock fidelities ploted with different approximations for the molecular Hamiltonian.



Real Material Simulations

First quantized approaches for quantum computers have recently been developed and are promising.



Recent advances have shown that a log(N) number of qubits can be used to simulate N plane waves

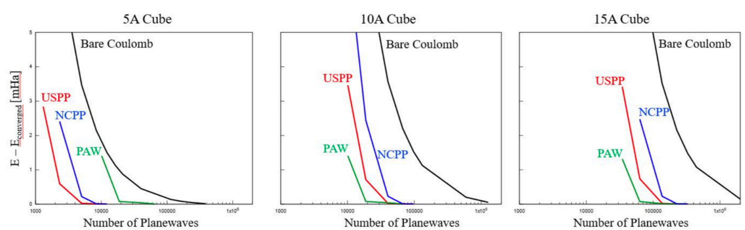
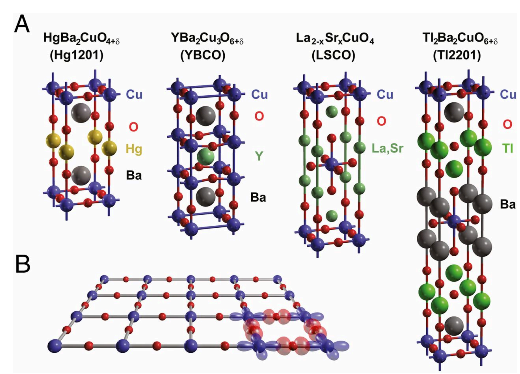


Figure 2. Planewave convergence of the hydrogen atom as calculated with planewave DFT codes. USPP are ultrasoft, NCPP is norm conserving, PAW are projected augment planewaves and Bare Coulomb is without pseudopotentials. The 4 decades labeled on the x-axis are 1000, 10,000, 100,000 and 1 million planewaves going from left to right.

Various mappings can provide approximate Hamiltonians suitable for simulation on near term hardware.

Resource estimates for both exact and approximate forms demonstrate that as quantum computing power increases, so will simulation accuracy.

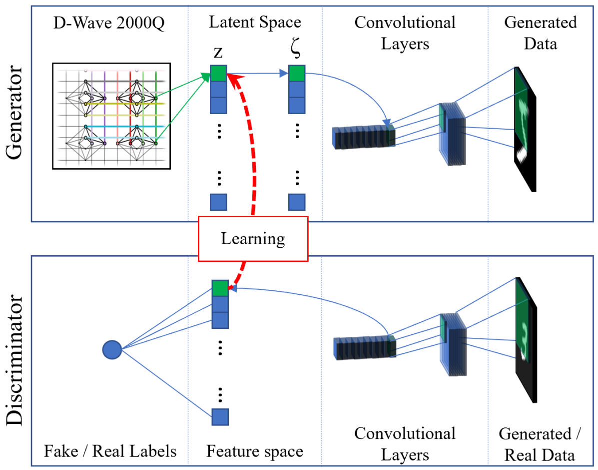
Many potential NASA applications include catalysis, battery materials, high temperature superconductivity, magnetic materials and more..

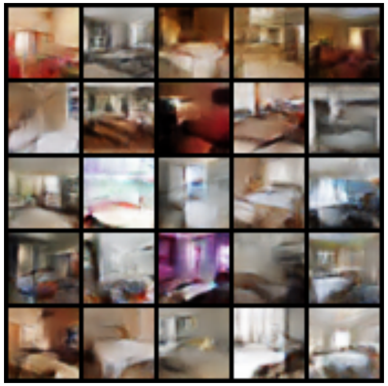


Neven Barišić et al. PNAS 2013

Quantum machine learning

Quantum-assisted associative adversarial network

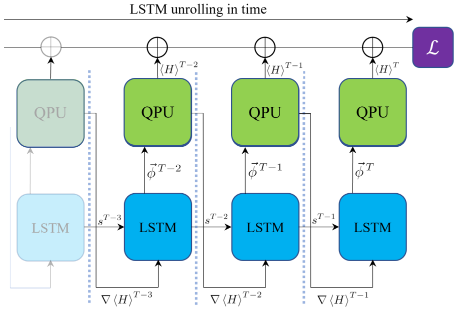




Scalable quantum-assisted GAN demonstrated on large continuous-valued color datasets (CIFAR Bedrooms)

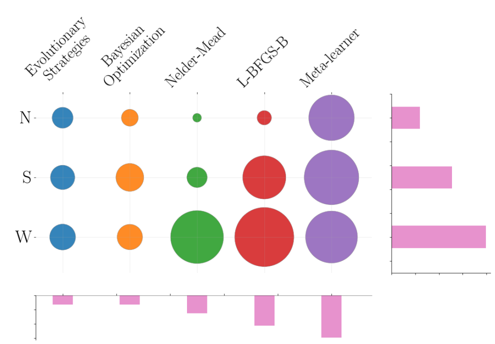
Max Wilson, Tad Hogg & Eleanor Rieffel, *Quantum-assisted associative adversarial network, arXiv:1904.10573*

Optimizing quantum heuristics with meta-learning



Learning to learn to optimize variational quantum algorithms with machine learning

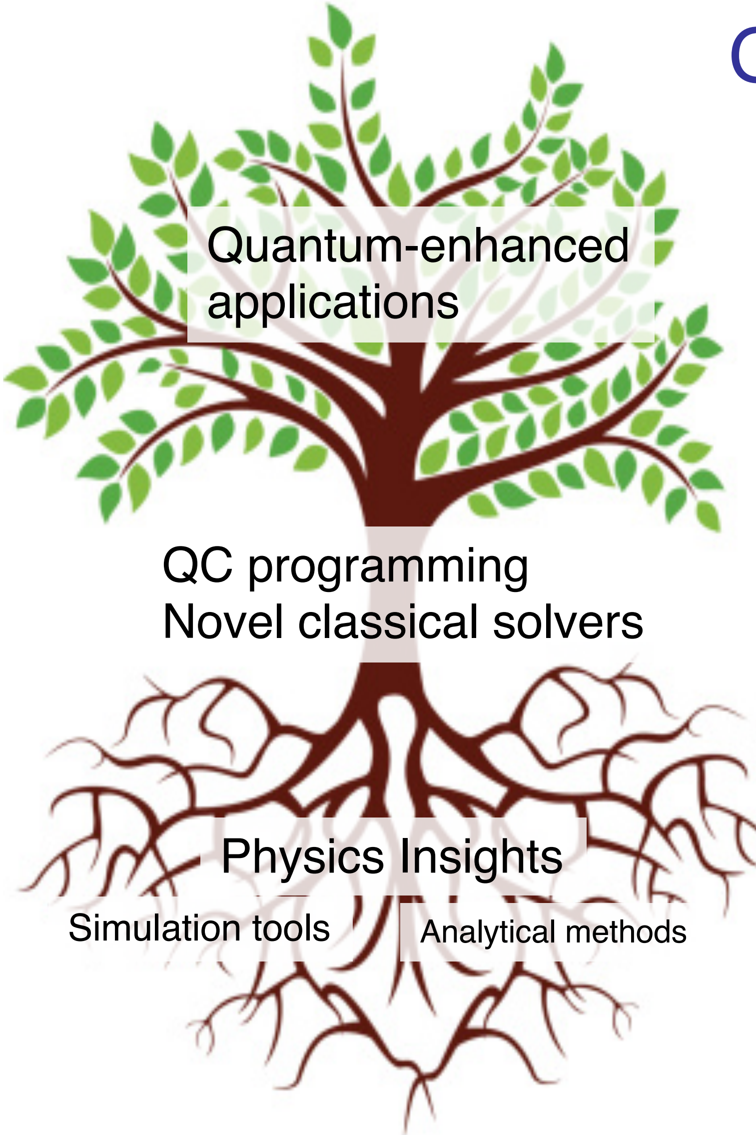
Better performance of meta-learner (optimizer) than closest comparable competitor Tested (L-BFGS)



More near-optimal solutions in a noisy environment

Max Wilson, Rachel Stromswold, Filip Wudarski, Stuart Hadfield, Norm M. Tubman, Eleanor Rieffel, *Optimizing quantum heuristics with meta-learning, arXiv:1908.03185*

Quantum Computing at NASA



Application focus areas

- **Planning and scheduling**
- **Robust networks**
- **Fault Diagnosis**
- **Machine Learning**
- **Material science simulations**

Programming quantum computers

- **Quantum algorithm design**
- **Mapping, parameter setting, error mitigation**
- **Hybrid quantum-classical approaches**
- **Compiling quantum algorithms to hardware**

QC → state-of-the-art classical solvers

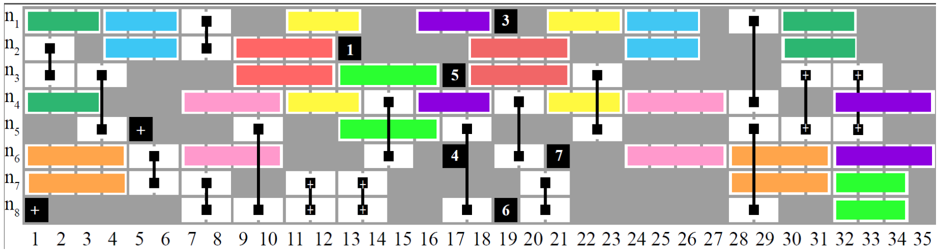
Physics insights into quantum algorithm and quantum hardware design

Compiling quantum algorithms to realistic hardware

Compilation of algorithms to a NISQ processor requires
- **Decomposition into native gates**
- **Qubit routing**

Qubit routing moves qubit states to locations where desired gates can be implemented
- **insert SWAP operations to handle limited connectivity**

Pioneered temporal planning for compilation to NISQ devices
- **Minimize makespan**
- **combined temporal planning with constrained programming**



Collaboration with

- Domain experts at NASA, utilizing state of the art temporal planners

- Rigetti, Google, and IBM hardware constraints

Currently extending beyond superconducting qubit devices, e.g. ion-trap quantum processors

Proven bounds on compilation, application to:
- **QAOA**
- **Quantum simulation of Fermionic systems**

D Venturelli, M Do, E Rieffel, J Frank., **Compiling quantum circuits to realistic hardware architectures using temporal planners**, *Quantum Science and Technology* (2018)

KEC Booth, M Do, JC Beck, E Rieffel, D Venturelli, J Frank , **Comparing and integrating constraint programming and temporal planning for quantum circuit compilation**, ICAPS (2018)

Bryan O'Gorman, William J. Huggins, Eleanor G. Rieffel, K. Birgitta Whaley, **Generalized swap networks for near-term quantum computing**, arXiv:1905.05118

Evaluating algorithm performance

Physics-inspired classical algorithms

State-of-the-art classical algs.

- Open-boundary Quantum Monte Carlo (QMC) [1]
- Population Annealing [2]
- Isoenergetic Cluster Method [3]
- Hybrid Cluster Method [4]
- Super-spin [5]

Increasingly Tailored

Collaboration with Katzgraber's group at TAMU

Unified Framework for Optimization (UFO)

[1] Z. Jiang, V. Smelyanskiy, S. Boixo & H. Neven, **Path-Integral Quantum Monte Carlo with Open-Boundary Conditions**, arXiv:1708.07117, 2017

[2] W. Wang, J. Machta & H.G. Katzgraber, **Population annealing: Theory and application in spin glasses**, PRA (2015)

[3] Z. Zhu, A.J. Ochoa & H.G. Katzgraber, **Efficient cluster algorithm for spin glasses in any space dimension**, PRL (2015)

[4] D. Venturelli, S. Mandrà, S. Knysh, B. O'Gorman, R. Biswas & V. Smelyanskiy, **Quantum optimization of fully connected spin glasses**, PRX (2015)

[5] S. Mandrà, Z. Zhu, W. Wang, A. Perdomo-Ortiz, H.G. Katzgraber, **Strengths and weaknesses of weak-strong cluster problems: A detailed overview of state-of-the-art classical heuristics versus quantum approaches**, PRA (2016)

Evaluation criteria

Analytically proven guarantees:

- Provable quantum speed-up (Grover)
- Strong quantum speed-up (Shor)

Numerical evaluation:

- Limited quantum speed-up
  - Compared with current best classical approach
- Limited Non-tailored quantum speed-up
  - Current best generic classical alg. not tailored to a particular problem
- Limited Tailored quantum speed-up
  - Current best classical alg., explicitly tailored to problem at hand

Mandra, Zhu, Want, Perdomo-Ortiz, Katzgraber, **Strengths and weaknesses of weak-strong cluster problems: A detailed overview of state-of-the-art classical heuristics vs quantum approaches**. *PRA* (2016)

Classical HPC simulation of quantum circuits

Advanced the state-of-the-art

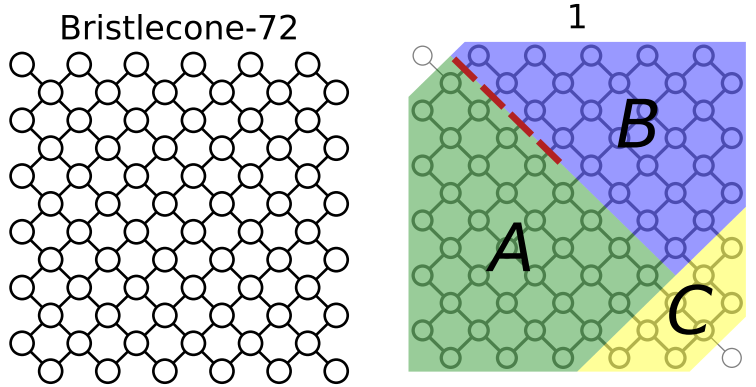
- **can simulate larger quantum circuits than any previous approach**
- **judicious use of cuts within a tensor network contraction**
- **HPC memory tricks and trade-offs**
- **can flexibly incorporate fidelity goal**

Largest computation run on NASA HPC clusters

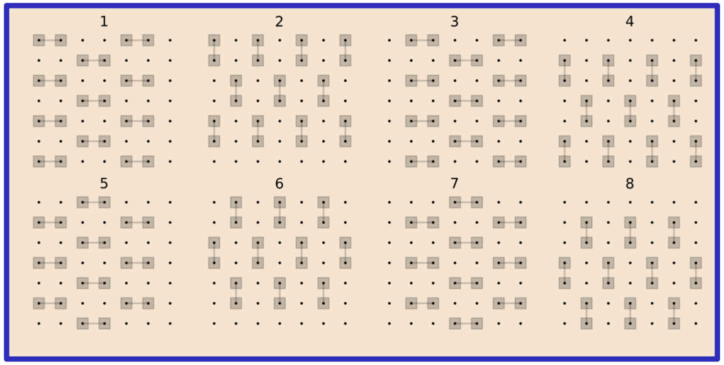
- **60-qubit subgraph, depth 1+32+1**
- **116,611 processes on 13,059 nodes, peak of 20 PFLOPS, 64% of max**
- **across Pleiades, Electra, Hyperwall**

Applications

- **quantum supremacy experiments**
- **benchmark emerging quantum hardware**
- **empirically explore quantum algorithms**



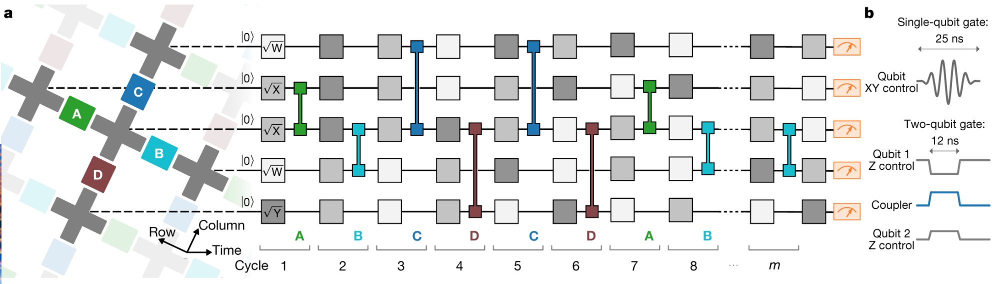
Computed exact amplitudes for 72 qubit Bristlecone random circuit, depth 1+32+1



Villalonga et al., ***A flexible high-performance simulator for the verification and benchmarking of quantum circuits implemented on real hardware***. NPJ Quantum Information 5, 1-16

Villalonga et al., ***Establishing the Quantum Supremacy Frontier with a 281 Pflop/s Simulation***, arXiv:1905.00444

Quantum Supremacy

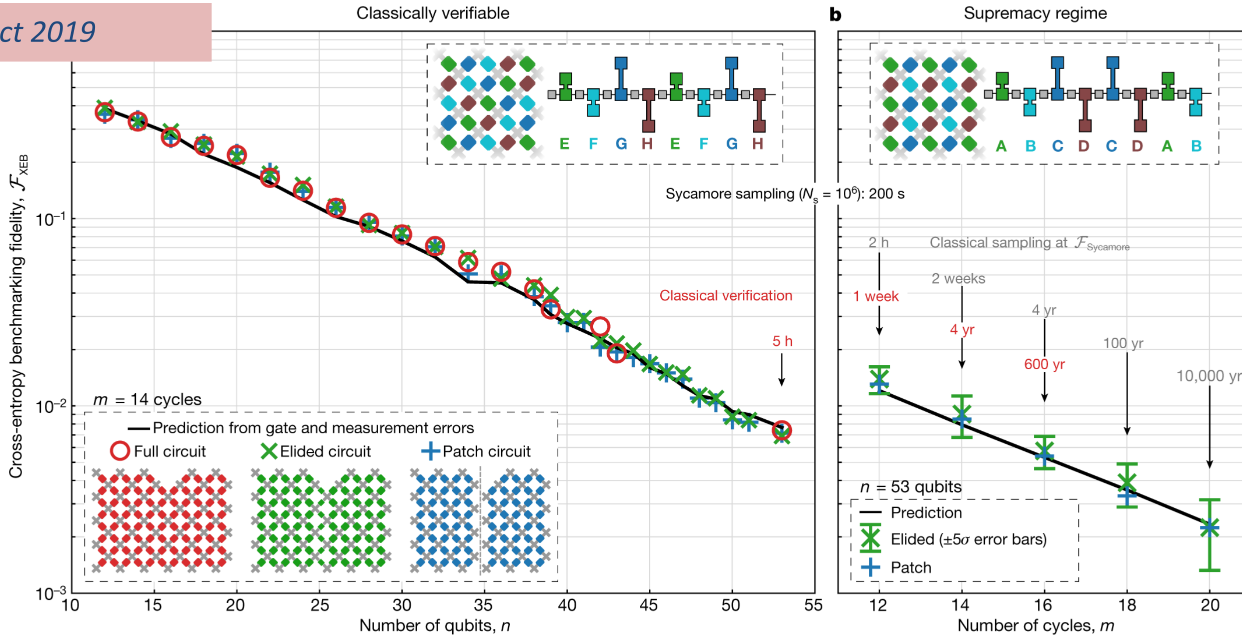


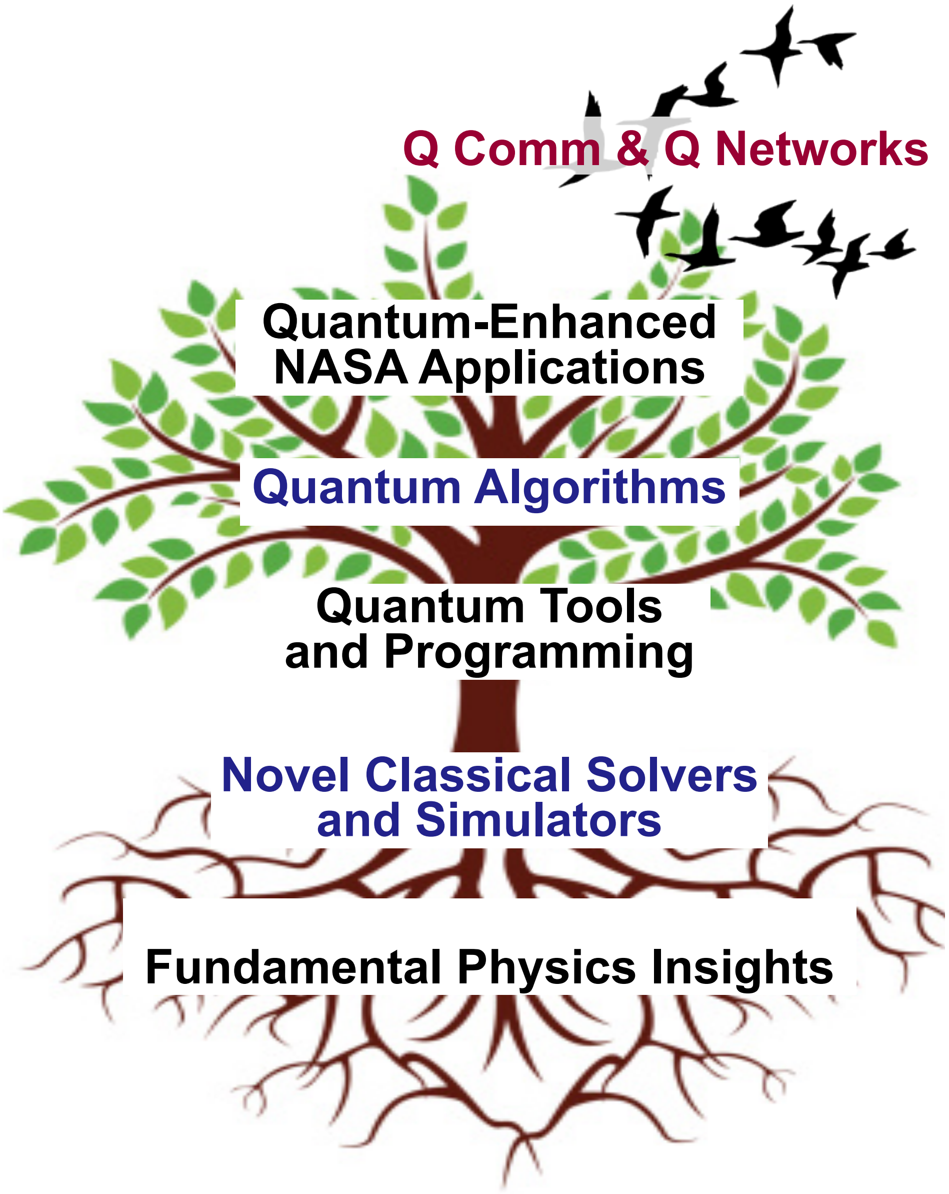
***Example random quantum circuit**. Every cycle includes a layer of single- and two-qubit gates. The single-qubit gates are chosen randomly from a set of three gates. The sequence of two-qubit gates follow a tiling pattern, coupling each qubit sequentially to its four neighbors.*

How do you verify a computation that no other hardware can do?
- check smaller version
- check pieces
- check variants that are simpler to simulate

24 Oct 2019

- Entering an era of unprecedented ways to explore quantum algorithms.
- Era of quantum heuristics.
- These explorations will broaden the known application of quantum computing.





Networking quantum processors enables larger quantum computations

Connecting classical and quantum processors supports hybrid methods

Connecting limited capability quantum devices to QCs enables delegated quantum computing

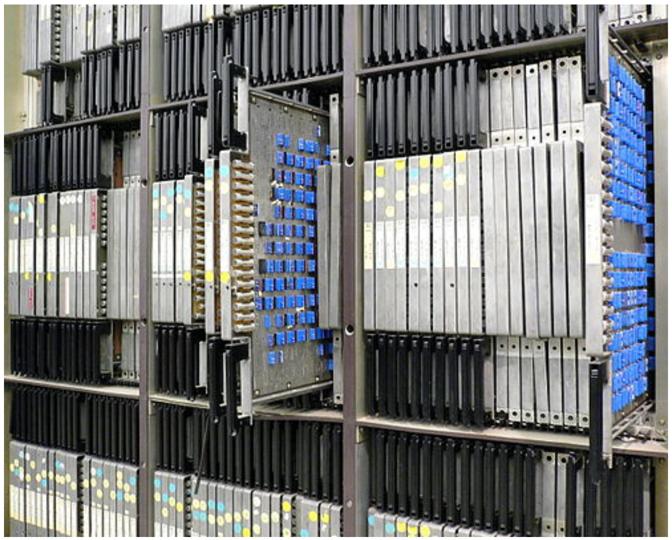
Verifiable QC enables client to determine if desired quantum computation has been performed

- Means to benchmark prototype quantum computing hardware
- Security applications in the long term

Blind quantum computing enables client to use QC without QC provider learning anything about computation

Envision a heterogeneous landscape, with a variety of quantum processors, with differing strengths

A Historical Perspective



NASA Ames director Hans Mark brought Illiac IV to NASA Ames in 1972

Illiac IV - first massively parallel computer

- **64 64-bit FPUs and a single CPU**
- **50 MFLOP peak, fastest computer at the time**

Finding good problems and algorithms was challenging

Questions at the time:

- **How broad will the applications be of massively parallel computing?**
- **Will computers ever be able to compete with wind tunnels?**

Take away points

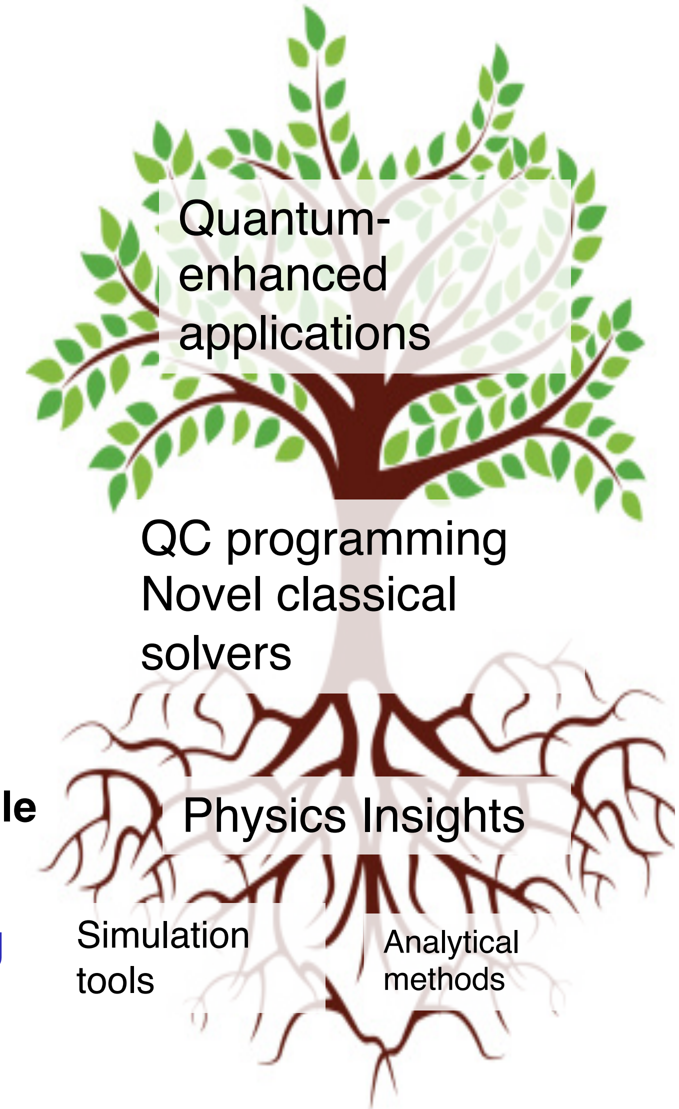
Deep connection between fundamental physics and computer science

- **How fast does nature let us compute?**
- **Many open questions remain**

The next years will be even more exciting!

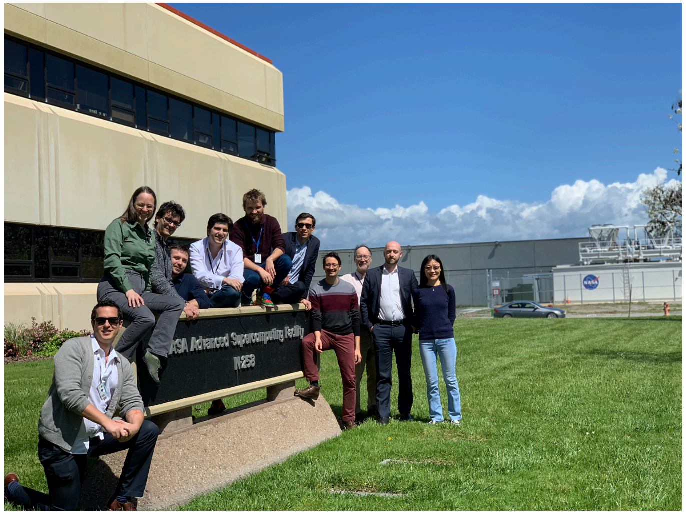
- **Quantum hardware improvements will support yet larger and more powerful computations**
- **Unprecedented opportunity to investigate quantum algorithms and quantum mechanisms on a larger scale**

Please talk with us about your most challenging computational problems!



NASA QuAIL Team

NASA Ames Research Center



Eleanor G. Rieffel, Stuart Hadfield, Tad Hogg, Salvatore Mandrà, Jeffrey Marshall, Gianni Mossi, Bryan O'Gorman, Eugeniu Plamadeala, Norm M. Tubman, Davide Venturelli, Walter Vinci, Zhihui Wang, Max Wilson, Filip Wudarski, Rupak Biswas, ***From Ansätze to Z-gates: a NASA View of Quantum Computing***, arXiv:1905.02860

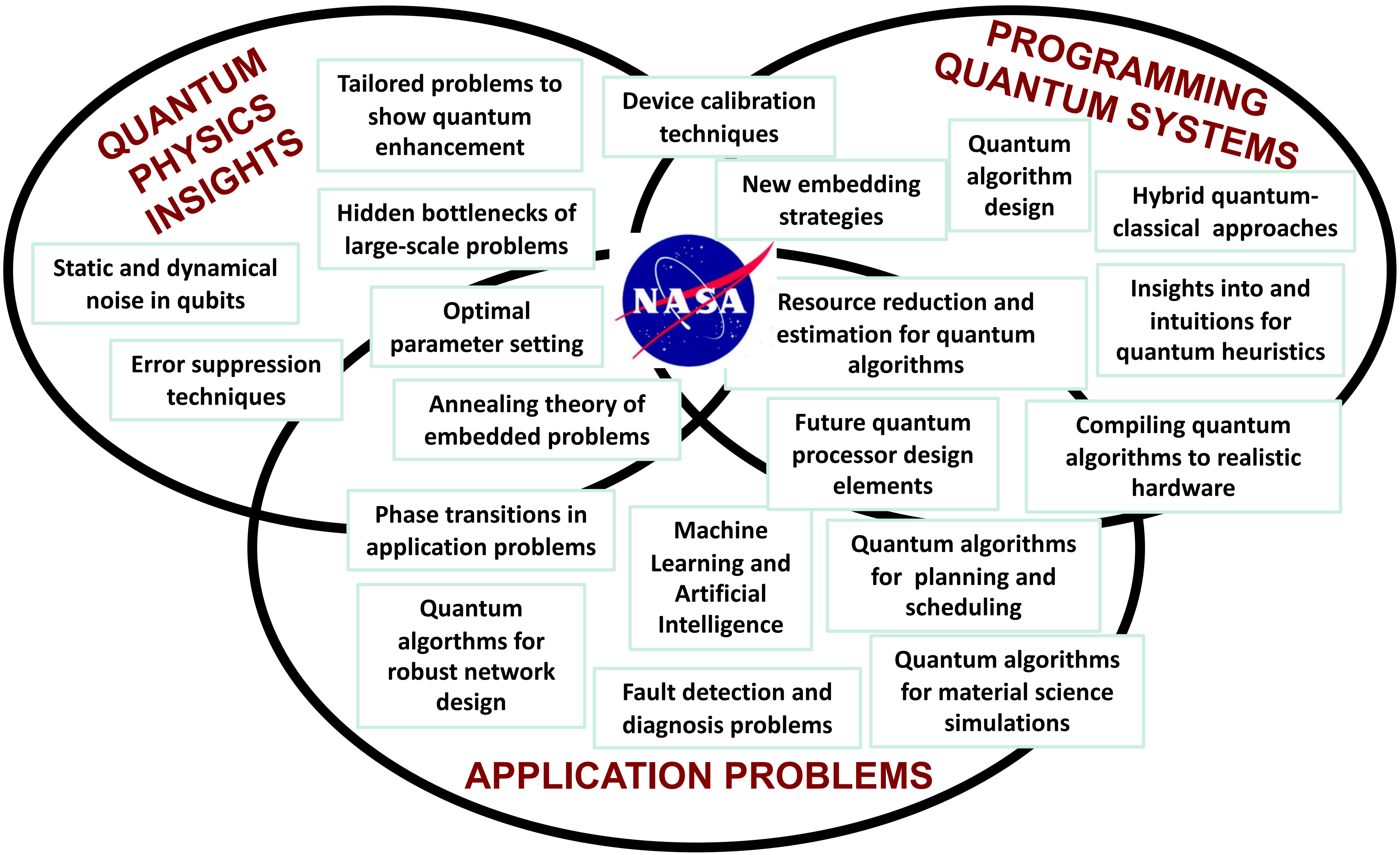
Rupak Biswas, Zhang Jiang, Kostya Kechezhi, Sergey Knysh, Salvatore Mandrà, Bryan O'Gorman, Alejandro Perdomo-Ortiz, Andre Petukhov, John Realpe-Gómez, Eleanor Rieffel, Davide Venturelli, Fedir Vasko, Zhihui Wang, ***A NASA Perspective on Quantum Computing: Opportunities and Challenges***, Parallel Computing, Volume 64, May 2017, p. 81-98, arXiv:1704.04836

National Aeronautics and Space Administration

Ames

Discovery Innovations Solutions

NASA Quantum Research Approach



NASA Quantum Research Approach